Diethylmalonic acid, di(2-isopropylphenyl) ester

Inchi: InChI=1S/C25H32O4/c1-7-25(8-2,23(26)28-21-15-11-9-13-19(21)17(3)4)24(27)29-22-16-12-10-14-20(22)18(5)6

InchiKey: CLZRYZDDEUORKX-UHFFFAOYSA-N

Formula: C25H32O4

SMILES: CCC(CC)(C(=O)Oc1ccccc1C(C)C)C(=O)Oc1ccccc1C(C)C

Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
gf	-104.70	kJ/mol	Joback Method
hf	-618.12	kJ/mol	Joback Method
hfus	38.92	kJ/mol	Joback Method
hvap	93.36	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	6.251		Crippen Method
mcvol	330.470	ml/mol	McGowan Method
pc	1223.41	kPa	Joback Method
rinpol	2485.00		NIST Webbook
rinpol	2485.00		NIST Webbook
tb	983.19	K	Joback Method
tc	1215.27	K	Joback Method
tf	566.13	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1076.98	J/mol×K	983.19	Joback Method
cpg	1091.69	J/mol×K	1021.87	Joback Method
cpg	1104.98	J/mol×K	1060.55	Joback Method
cpg	1116.93	J/mol×K	1099.23	Joback Method
cpg	1127.61	J/mol×K	1137.91	Joback Method
cpg	1137.11	J/mol×K	1176.59	Joback Method
cpg	1145.51	J/mol×K	1215.27	Joback Method
dvisc	0.0002782	Pa×s	566.13	Joback Method

dvisc	0.0001366	Pa×s	635.64	Joback Method
dvisc	0.0000772	Pa×s	705.15	Joback Method
dvisc	0.0000483	Pa×s	774.66	Joback Method
dvisc	0.0000327	Pa×s	844.17	Joback Method
dvisc	0.0000234	Pa×s	913.68	Joback Method
dvisc	0.0000176	Pa×s	983.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369984&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume